Competition between d-wave superconductivity and antiferromagnetism in the 2D Hubbard model

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We study the competition of antiferromagnetism and d-wave superconductivity at zero-temperature in the two-dimensional Hubbard model using Cellular Dynamical Mean Field Theory. The interplay between the two phases depends strongly on the strength of the correlation. At strong coupling ($U \geq 8t$) the two phases do not mix, and a first-order transition takes place as a function of doping between two pure phases. At weak-coupling ($U \leq 8t$) the two order parameters coexist within the same solution in a range of doping and the system smoothly evolves from the antiferromagnet to the superconductor. When the transition between the superconducting and the antiferromagetic phases is of the first-order, it is accompanied by a phase separation.

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The competition of d-wave superconductivity (dSC) and antiferromagnetism (AFM) in the repulsive Hubbard model is a central problem in the theory of strongly correlated electron systems. In the cuprate high temperature superconductors dSC emerges by doping a parent compound which has AFM long-range order. Hence, the question of whether the proximity to AFM is detrimental or favorable for superconductivity has been debated for nearly twenty years but no clear consensus has been reached. For a recent review of these topics see Ref. [1].

dSC and AFM can be clearly identified as the leading instabilities in weak-coupling functional renormalization group of the Hubbard model[2], but this method is unable to describe the competition between the two phases at zero temperature. On the other hand, a number of approaches predicts that the transition between the AFM and the dSC takes place through an intermediate phase where both order parameters are finite. For example variational wavefunctions of the Gutzwiller type give rise to dSC upon doping both in the Hubbard and t-J models[3]. However natural extensions of these wavefunctions incorporating the possibility of AFM [4] result in a phase diagram where the stable state is a homogeneous mixture of dSC and AFM. The slave boson approach to the Resonating Valence Bond (RVB) theory finds that the dSC state has the lowest energy upon doping in a manifold of degenerate RVB states at half filling [5]. However, when AFM is included into the Hartree-Fock slave-boson decoupling [6], a mixture of dSC and AFM is stabilized. Finally the variational cluster perturbation theory approach with small cluster sizes find a mixture of superconductivity and AFM away from half filling.[7, 8]

Dynamical Mean-Field Theory (DMFT)[9], and its cluster extensions [10] allow us to reexamine the competition between dSC and AFM from an unbiased perspective in the sense that all the broken symmetries with order parameters that fit within a given cluster are treated on the same footing. Furthermore, by having a Weiss mean-field containing both anomalous and normal dynamical components, one expects to avoid spurious broken symmetries that can appear in variational treatments with restricted variational freedom.

We consider the two-dimensional Hubbard model

$$H = -t \sum_{\langle i,j \rangle,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i, \tag{1}$$

where $c_{i,\sigma}$ ($c^{\dagger}_{i,\sigma}$) are destruction (creation) operators for electrons of spin σ, $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the density of σ-spin electrons, t is the hopping amplitude, U is the on-site repulsion and μ the chemical potential.

In CDMFT we select a cluster of N_c sites, and we map the lattice model onto an effective action for the cluster, which hybridizes with a bath. A self-consistency equation determines the spectral function of the bath, also called dynamical Weiss field. For practical purposes, it is useful to resort to a Hamiltonian formulation, where the quantum fluctuations on the cluster are realized by hybridization with a conduction bath. This leads to a cluster-impurity Hamiltonian of the form

$$\mathbf{H}_{ACI} = H_c + \sum_{k\sigma} \varepsilon_k \, a^{+}_{k\sigma} a_{k\sigma} + \sum_{k\mu\sigma} V_{k\mu\sigma} \, a^{+}_{k\sigma} c_{\mu\sigma} + h.c. + \sum_{k\mu\sigma} V^{S}_{k\mu} \, a^{\dagger}_{k\uparrow} c^{\dagger}_{\mu\downarrow} + h.c., \tag{2}$$

where H_c contains the terms of the Hamiltonian which belong to the cluster, the index $\mu = 1, \ldots, N_c$ labels the cluster sites, and $a_{k\sigma}$ are auxiliary bath degrees of freedom. Here, since we are interested in superconductivity, there is an "anomalous" hybridization term which creates and destroys a pair in which one electron is on the

cluster, and the other in the bath. The cluster-impurity model is still a non-trivial many-body problem, which we solve using exact diagonalization (ED). This approach allows us to obtain zero-temperature results [11, 12], and it has been successfully applied to the normal[13] and superconducting state[14, 15] close to Mott insulators. The use of ED requires a finite Hamiltonian matrix. Hence the sums in Eq. (2) are limited to a discrete set of values $k_i = 1, \dots N_b$. This truncation is the only approximation introduced in the ED approach to CDMFT. In practice, at each DMFT iteration, one determines the Anderson parameters that better describe the Weiss field obtained through self-consistency. This requires the minimize a suitably defined distance between the Weiss field and its discretized counterpart. The details of the implementation are described in Ref. [12].

In this work we always consider a two dimensional $N_c = 4 = 2 \times 2$ plaquette as a minimal cluster where both AFM and dSC are possible, and a bath of $N_b = 8$ sites. The same cluster has been studied at finite temperature within a different cluster extension of DMFT in Ref. [16]. Even with this small cluster, the number of parameters to minimize is quite large. Since we expect that the main tendencies of the 2D Hubbard model are AFM and dSC, we found it useful to restrict, as a *preliminary* step to solutions with one or the other broken symmetries. Therefore we introduced "constrained" parametrizations with significantly reduced number of parameters in which only pure AFM or pure dSC solutions are allowed. This allows us to determine in a much faster way the regions of the phase diagrams in which the two pure broken-symmetry phases exist at $T = 0$. As a second step, we reintroduced the full parametrization, using the pure solutions defined above as starting points of the iterations, but adding small perturbations with defined symmetries. In this way, we have been able to verify the *local* stability of the pure solutions one with respect to the other. With this second step, we tested the possibility of coexistence between AFM and dSC. Finally, we added small perturbations with other symmetries and we also considered the case with no definite symmetry.

We performed calculations as a function of hole doping $\delta = 1 - n$ ($n = 1/N_c \sum_{i=1,Nc} \langle n_i \rangle$ being the density per site) for different values of U/t ranging from weak to strong coupling, and we applied the protocol defined above. We first limited ourselves to pure solutions and we identified the regions of doping in which the pure AFM and dSC solutions exist. The evolution of the staggered magnetization in the AFM phase $m = \langle \sum_i (-1)^i (n_{i\uparrow} i - n_{i\downarrow}) \rangle$ and of the dSC order parameter in the superconducting phase $\Delta = \langle \sum_i c_{i,\uparrow} c_{i+,\downarrow} - c_{i,\uparrow} c_{i+y,\downarrow} \rangle$ as a function of doping is shown for $U = 4t, 8t, 12t$ and $16t$ in Fig. 1. At half-filling $\delta = 0$, the magnetization is an increasing function of U/t in the whole interaction range. When we dope the system away from half filling, m decreases and goes to zero at a relatively large doping $\delta_{afm} \simeq 0.14 - 0.16$, which does not depend strongly on the value of U, but has larger values for intermediate coupling. The behavior of order parameter of the pure dSC solution is richer. In the weak-coupling case $U/t = 4$, Δ evolves in a way similar to m, namely it is maximum at zero doping and monotonically decreases as the hole concentration grows. The situation changes for large repulsion values, when the repulsion is large enough to make the system a Mott insulator even in the absence of any form of magnetic long range order. In this range Δ vanishes when we approach the Mott insulator at zero doping, then it rises to a maximum and eventually decreases for larger doping. Hence for $U/t = 8, 12$ and 16, the superconducting order parameter has the dome-like shape characteristic of the superconductivity taking place near a Mott transition, such as in the high temperature superconductors. The position of the "optimal doping" is around $x = 0.1$, and it weakly increases as U/t increases. The maximum value of the dSC order parameter basically scales with $J = 4t^2/U$ for the large values U/t, as expected in the treatments where the superexchange interaction is the origin of superconductivity as in the slave boson method. Our pure dSC solution is similar to that reported earlier in Ref. [14].

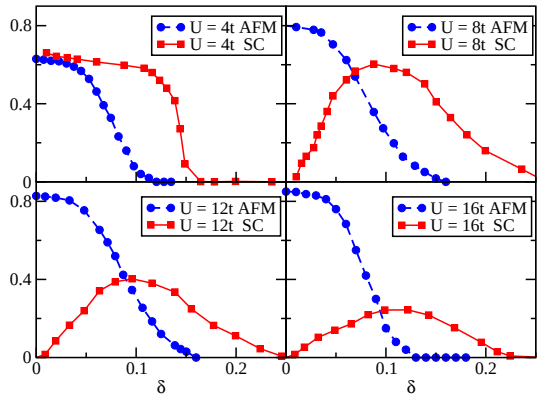

FIG. 1: (Color online) AFM (blue dashed line with squares) and dSC (red solid line with circles) order parameters as a function of doping for four values of the repulsion $U/t = 4, 8, 12$ and 16. The dSC order parameter is multiplied by a factor 10 for graphical purposes.

We now turn to the competition between the two phases. For all the parameter sets considered above we relaxed the parametrization, allowing for deviations from pure AFM or dSC order. As mentioned above, we first considered the local stability of the two solutions. Therefore, in the regions where two solutions exist, we started the iterations from one of the pure solutions, adding a small perturbation in the competing channel. The outcome of this perturbation strongly depends on the value of U/t. For $U/t = 4$, the AFM and dSC solutions, the small perturbations are stabilized by the CDMFT itera-

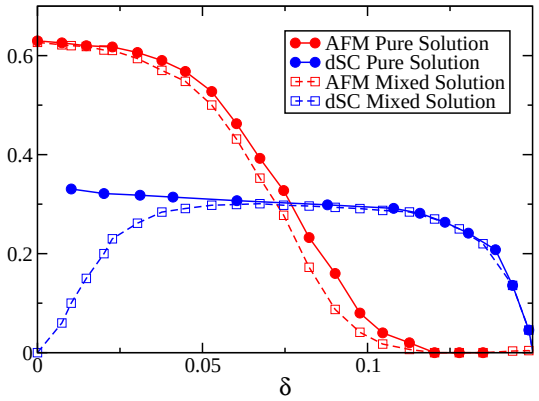

FIG. 2: (Color online) AFM and dSC order parameters as a function of doping for four $U/t = 4$. We compare the values of the order parameters in the pure solutions (full line and filled circles) with the values in the mixed solution (dashed line and open squares). The dSC order parameter was multiplied by a factor 10 for graphical purposes.

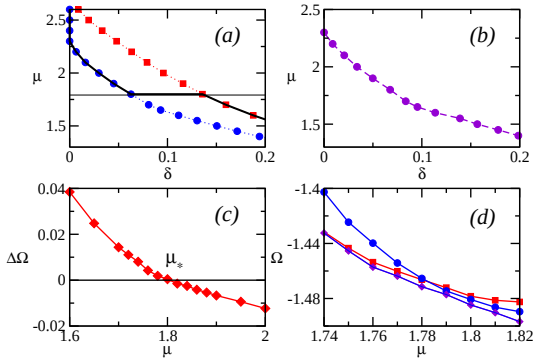

FIG. 3: (Color online) Chemical Potential as a function of doping for $U = 16t$ [panel (a)] and $U = 4t$ [panel (b)]. In the former case the red curve with dots is the AFM solution, the blue one with squares the dSC, and the black line is the actual solution as a function of doping. In panel (b) only the stable mixed solution is shown. Panel (c) shows the difference between the grandcanonical energies of the AFM and dSC, and Panel (c) compares the energy of the AFM (red), of the dSC (blue) and of the mixed solution (violet).

tions and a mixed-phase with both order parameters finite is stabilized. In Fig. 2, we show the value of the two order parameters in the mixed state for $U/t = 4$, compared with their values in the starting pure phases. The superconducting component develops for small doping, and grows quite rapidly, while the staggered magnetization is only slightly smaller than the value of the pure AFM solution. For larger doping the dSC order parameter in the mixed state collapses on the pure solution, and the AFM order parameter becomes slightly smaller. We will see in the following that the mixed state is not only a solution spontaneously developed by the iterations, but it also has a lower energy than the pure ones. A similar behavior has been found in static mean-field [17].

For large $U/t = 12, 16$, the two solutions (pure dSC and pure AFM) are found to be stable against the perturbations described above: a small dSC(AFM) perturbation of the AFM(dSC) state disappears as the iterative procedure goes on, signaling that the two states are in direct competition which each other and cannot be connected. For $U/t = 8$ the situation is intermediate: A small mixture between the two solutions takes place, but the magnitude of the "minority" order parameter is found to be really small, basically of the same order of the truncation error of the ED calculation. For this reason we can not judge whether this value of U lies in the weak-coupling or in the strong-coupling regime, but we can surmise it is close to the boundary between the two regimes.

The third step of our approach perturbs the previously obtained solutions with Weiss fields with other symmetries (e.g., a $d + is$ superconductivity) or with perturbations with no definite symmetries. Regardless the value of U/t, we find that these perturbations all vanish through the iterative procedure. Thus we conclude that we only have pure AFM, pure dSC and mixed AFM+dSC as locally stable solutions of the CDMFT equations on a two by two plaquette. To establish which solution is the globally stable one we compute their grandcanonical potential at zero temperature $\Omega = \langle H - \mu N \rangle = \langle H_{kin} \rangle + \langle H_{int} \rangle - \mu \langle N \rangle$. The interaction term is given by the expectation value of the double occupancy on the cluster sites, while the kinetic energy requires the knowledge of the lattice Green's function $G(k, \omega)$, as $E_{kin} = \sum_k \epsilon_k G(k, \omega)$, where ϵ_k is the non-interacting dispersion. Different schemes have been proposed to extract lattice properties from cluster ones. Here we use the approach of Ref. 18, where the lattice self-energy is obtained by periodizing the cluster self-energy, but we have also checked that alternative methods [7, 14, 19] do not qualitatively affect the qualitative phase boundaries and the nature of the transitions, and that the quantitative differences are not large.

For $U/t = 4$ the mixed phase has lower Ω than the two pure phases, and it is thermodynamically stable since the chemical potential is a monotonic function of the doping (panels (b-d) of Fig. 3). For $U/t = 12$ and 16, the comparison of the energy determines the range of absolute stability of the two mutually exclusive solutions, as shown in panel (c) of Fig. 3, where the difference $\Delta\Omega = \Omega_{dSC} - \Omega_{AFM}$ is plotted for $U/t = 16$. $\Delta\Omega$ becomes zero at $\mu = \mu^*$, where the system jumps from one phase to the other through a first-order transition. the curve of $\Omega(\mu)$ has the wrong curvature (corresponding to negative compressibility) in an interval. The system is therefore no longer stable in a uniform phase, and it phase separates. This is clearly seen in the plot of the chemical potential as a function of doping, where at μ^*

the system turns from AFM to dSC, leaving a window of forbidden dopings.

In conclusion, we have studied the competition of AFM and dSC within the two-dimensional Hubbard model at zero temperatures using the CDMFT, an unbiased approach which treats both forms of order on the same footing. Using an ED solver, we have been able to span a wide range of correlation values, from $U/t = 4$ to $U/t = 16$, and followed the evolution of the two phases. At weak-coupling the AFM and dSC coexist in a single phase with two order parameters in agreement with the results of a weak coupling analysis [20]. In the pure solutions with a single order parameter, Δ and m are maximum at half-filling and decrease as a function of doping. Allowing for a simultaneous ordering suppresses the dSC order parameter in favor of the AFM one. For large U we find that there is no mixture and AFM and dSC exist as pure phases. A first-order transition as a function of doping occurs between the two phases, accompanied by a phase separation. Hence AFM and dSC exclude each other for large U. It is therefore possibile to follow the metastable pure d-wave state at small doping to study the approach towards the Mott insulator. This will be explored in a forthcoming publication [21]. While many properties of the pure superconducing phase are correctly described by simpler methods such as Gutzwiller variational wavefunctions or slave boson techniques, these methods are not able to describe the stability against admixture of magnetism which requires an accurate description of both ordered phases. In fact, the abrupt first order phase transition between dSC and AFM can only been obtained with fairly sophisticated trial wavefunctions [22] or through the bond operator method, which captures some aspects of the CDMFT with static expectation values [20]. It is interesting to notice, that a condition for the Hubbard model to have SO(5) symmetry requires to be in the tricritical region where the competition between AF and dSC switches to an homogeneous mixture of the two order parameters [1]. In our calculations this occurs in the interesting intermediate coupling regime of $U \approx 8t$.

We emphasize here that CDMFT is designed to provide the best possible description of the dynamics associated with short-range correlations. For this reason we restricted our study to homogeneous states. CDMFT indicates that the pure Hubbard model should display phase separation in agreement with many other methods [23]. These tendency can be enhanced or eliminated by including more realistic features such as longer range interactions or hoppings, that may lead to more general real-space patterns such as stripes. This study clearly requires large clusters, or a long wavelenght Landau-Ginzburg approach, which could exploit the CDMFT 2×2 results as an input for determining the effective parameters. On the other hand, the different nature of the interplay of AFM and dSC in weak and strong coupling pointed out here is expected to be a very robust feature captured by our treatment of the Hubbard model. Furthermore, we expect that the basic energetics will have a weaker dependence on additional interactions such as the coupling to phonons that might be required for a realistic modeling of a specific correlated material.

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